A Perspective for Recognizing Discreteness distinctly from Continuum: Validity of Point Dipole Approximation to Set the Distance Scale.

The Context for this Contribution

Even though discreteness and continuum are terms frequently used and defined so often, within a homogeneous medium when there is a necessity to consider discrete region and a continuum, it is usually only a diffused boundary which can be attributed demarking the two regions. Most often it is not necessary to look for a quantitative measure for a distinct demarcation. In the article by this author, "Magnetized Material: Contributions within Lorentz Ellipsoids" in the Indian Journal of Physics, Vol 79(9), p-985-989 (2005) it has been pointed out that the HR PMR studies have provided an evidence that NMR measurements can yield much better insights into the detailed material aspects than till now recognized for from the experimental results combined with simple simulations. In particular it was pointed out for the first time because of the questions which arose during Shielding Tensor measurements, a way could be found to quantitatively find a distinct boundary line for carving out **Inner** (semi micro) **Volume Element** I.V.E which is treated discretely within the homogeneous medium while the remaining part is treated as a continuum.

The Lorentz Sphere had been known since early days of magnetic materials but this clarity could come about aided by HR PMR measurements recently.

This aspect has a lot to clarify on the conflicts which chemists encounter while addressing the field distributions, magnetic moments and its contribution to induced fields. An effort is being made to provide illustration and a discussion on this aspect in this presentation.

ABSTRACT

A Perspective for Recognizing Discreteness distinctly from Continuum: Validity of Point Dipole Approximation to Set the Distance Scale.

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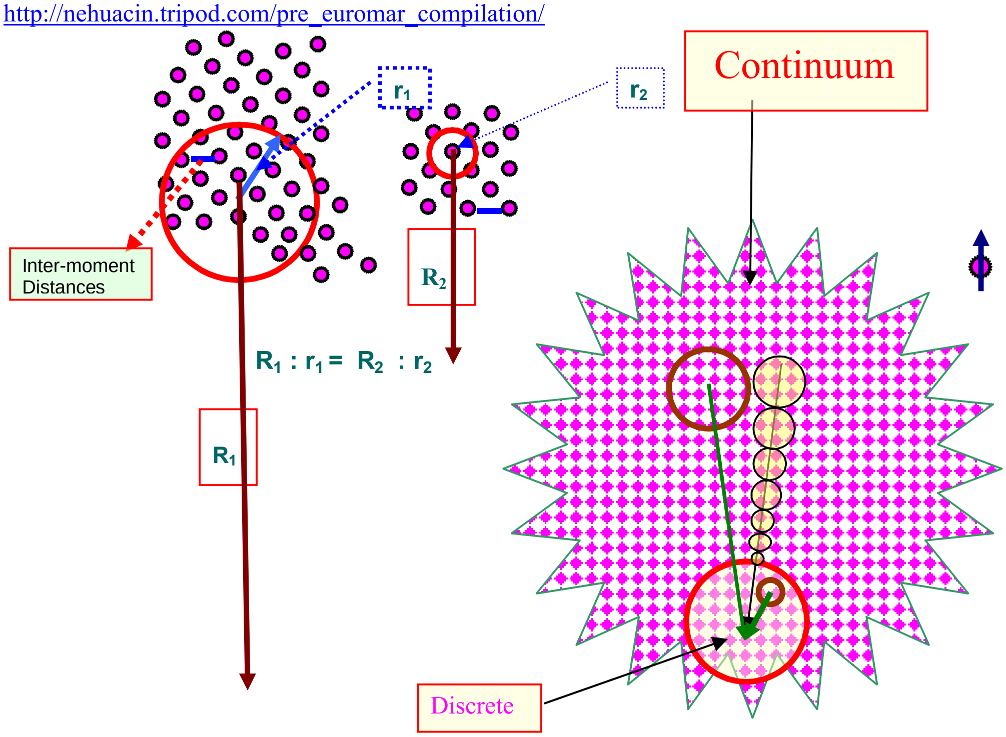
The materials in any state of matter are made up of discrete units and depending upon when and how it becomes relevant and possible to count the units as individual entities is when the term discreteness is applicable. However, mostly when ensemble properties are considered and the material as a bulk is what can be tangible for consideration, the term continuum is applicable. But there are instances when the given specimen has to have within itself demarcations as discrete region and continuum. Such are the contexts when it becomes necessary to consider critically and quantitatively a criterion to draw a boundary line within the medium which is otherwise homogeneous and does not have any distinctions characteristically associated with the constituents or the way the constituent units are organized within the material medium which in this context can be special arrangements and the inter unit distances.

The example of a single crystal of organic molecule would present the disposition of the molecules as described above; and, the applicability of magnetic point dipole model for induced field values at specified sites within the single crystal specimen would be clarifying the extent to which the material has to be considered as discrete or as a continuum. This subject of the point dipole approximation and its validity in the contexts of chemist's use in interpreting spectroscopic results has been pointed out in the references 1-4 cited below.

It would be further elucidated that the magnitude of the susceptibility of the molecular unit, the intermolecular distance, and the distance of the specified site from the contributing units determines where the demarcation can be located between 'discrete' region and the 'continuum'. With typical values for the quantities the trends would be illustrated as graphical results, and diagrammatic illustration of the relative distances within the specimen and the related properties to together with the graphical results would be presented to comprehend the terms and defining boundary lines when it is necessary. A typical diagram which would be part of the illustration is displayed below.

1. http://www.geocities.com/saravamudhan1944/crsi_6nsc_iitk.html
2. http://www.geocities.com/inboxnehu_sa/crsi_nsc8_iitb.html
3. http://www.angelfire.com/art3/saravamudhan/iitm_crsi_ismar_ca98.html
4. http://nehuacin.tripod.com/pre_euromar_compilation/



INTRODUCTION

As described in the Section -3 of the article in http://nehuacin.tripod.com/pre_euromar_compilation/id1.html the material is divided into a region where the contents are treated as discrete entities and the remaining part where the material is treated as a continuum. For qualitative hypothetical purposes it had not been necessary to know here exactly the boundary line exists for such demarcation.

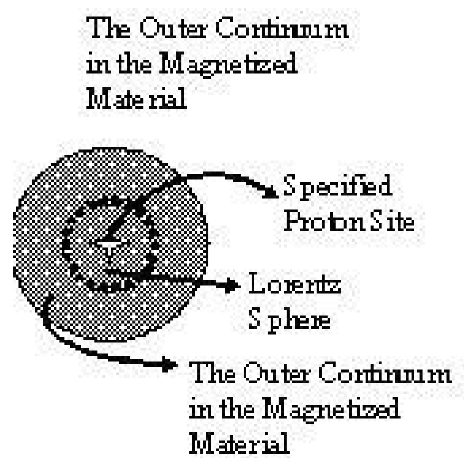


Fig.2. The hypothetical division of the spherical sample for consideration from the perspectives material medium

As pointed out in the publication Indian Journal of Physics, Vol.79(9), p 985-989 (2005) entitled “Magnetized Materials: Contributions Inside Lorentz Ellipsoids” it was by the requirements which arose due to HR PMR measurements in single crystals, it was possible to precisely demarcate the two regions within the material medium.

INTRODUCTION: Contd.

By looking into this possibility more critically, it could be discerned that such a result as reported in SHEET-1 became possible because of the trends of convergence of the sum of contributions calculated by discrete summation. This aspect is particularly appealing to be elucidated for the conceptual clarifications to chemists. Thus the details of these trends of summing using the point-dipole approximation from near to far around a site is presented to enable the chemists to rationalize similar trends which may arise in several other contexts in chemistry.

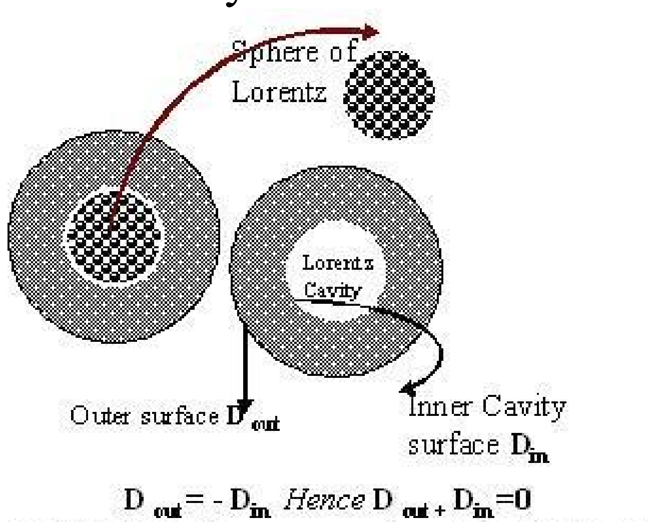
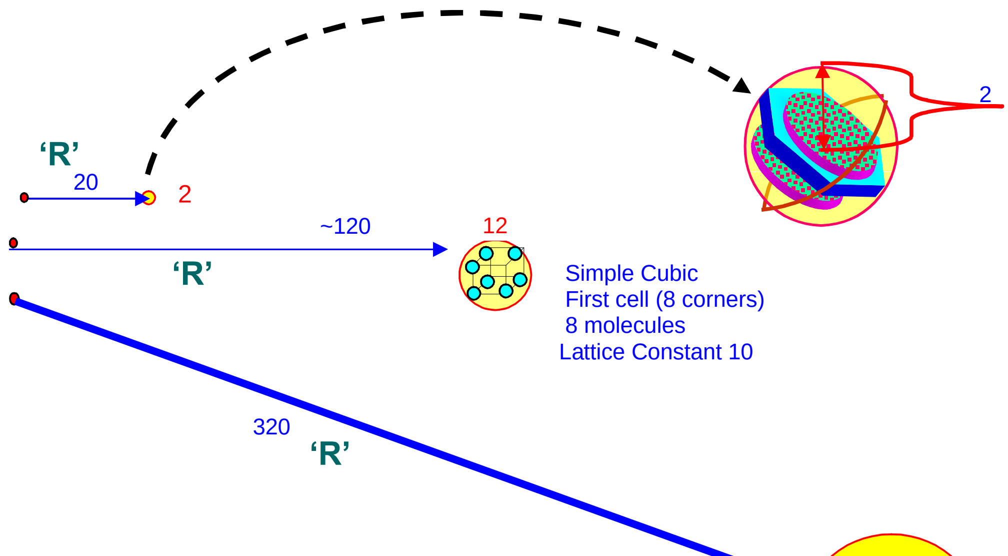
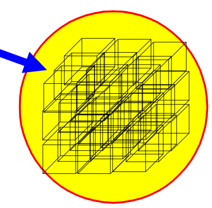


Fig.3. Explaining the consequence of zero induced field inside the spherical specimen. The D with of a subscripts stand for the demagnetization factors of thecorresponding boundary surfaces-inner & outer

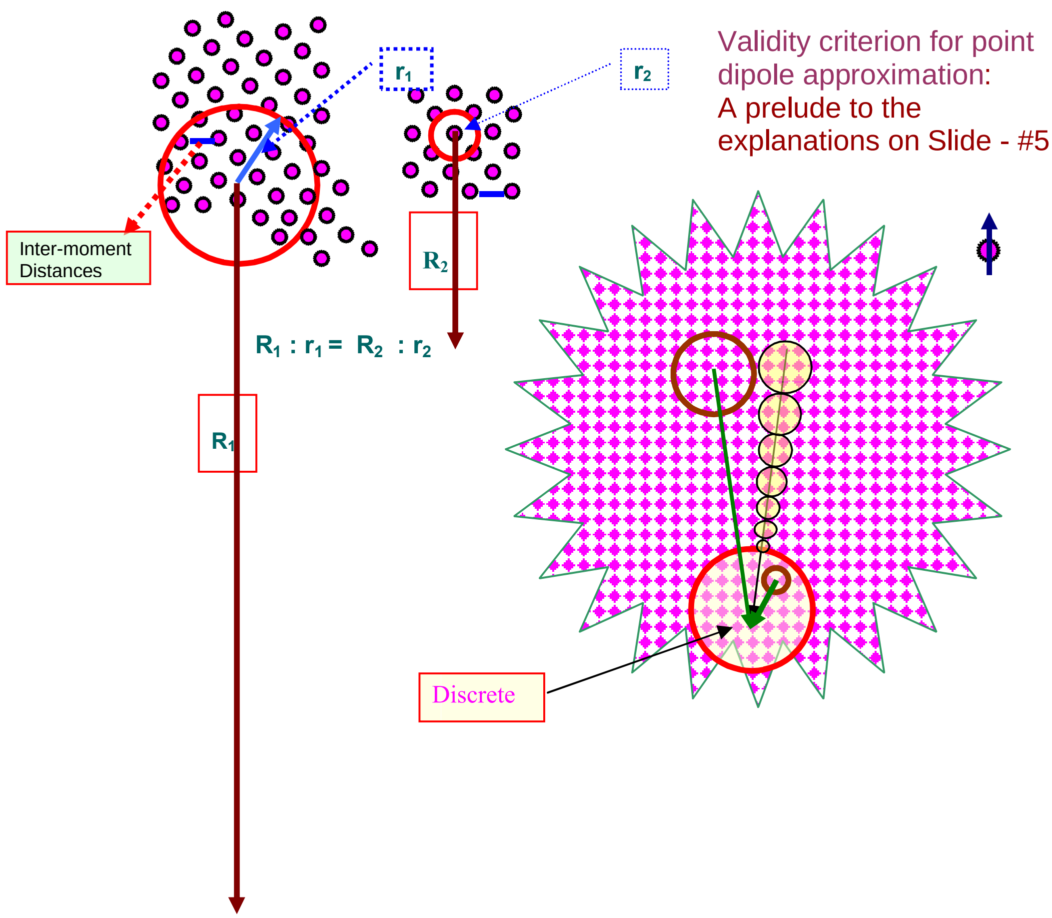
In the next sheet the comparative values of distances encountered are illustrated.

Comparative Typical Distance Values





. This sheet depicts the comparative situation for molecular sizes, intermolecular distances with respect to a distance 'R' from a fixed distant point



The Illustration below depicts the procedure for the Summation using the equation for the point dipole approximation. The equation used is as below:

$$\sigma = \frac{\chi}{R^3} - \frac{3 \bullet \cos^2(\theta) \bullet \chi}{R^3}$$

Where χ is the susceptibility tensor, R is the distance to the dipole, and θ is the angle which the distance vector makes with the magnetic field direction.
The tensor-expanded form of the equation is depicted below.
For

2. Calculation of induced field with the Magnetic Dipole Model using point dipole approximations.

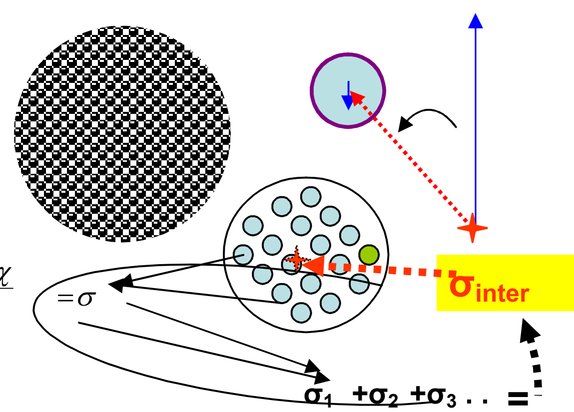
Induced field Calculations using these equations and the magnetic dipole model have been simple enough when the summation procedures were applied as would be described in this presentation.

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} = \frac{\begin{bmatrix} \chi_{xx} & \chi_{xy} & \chi_{xz} \\ \chi_{yx} & \chi_{yy} & \chi_{yz} \\ \chi_{zx} & \chi_{zy} & \chi_{zz} \end{bmatrix}}{r^3} - \frac{3 \bullet \begin{bmatrix} xx & xy & xz \\ yx & yy & yz \\ zx & zy & zz \end{bmatrix} \bullet \begin{bmatrix} \chi_{xx} & \chi_{xy} & \chi_{xz} \\ \chi_{yx} & \chi_{yy} & \chi_{yz} \\ \chi_{zx} & \chi_{zy} & \chi_{zz} \end{bmatrix}}{r^5}$$

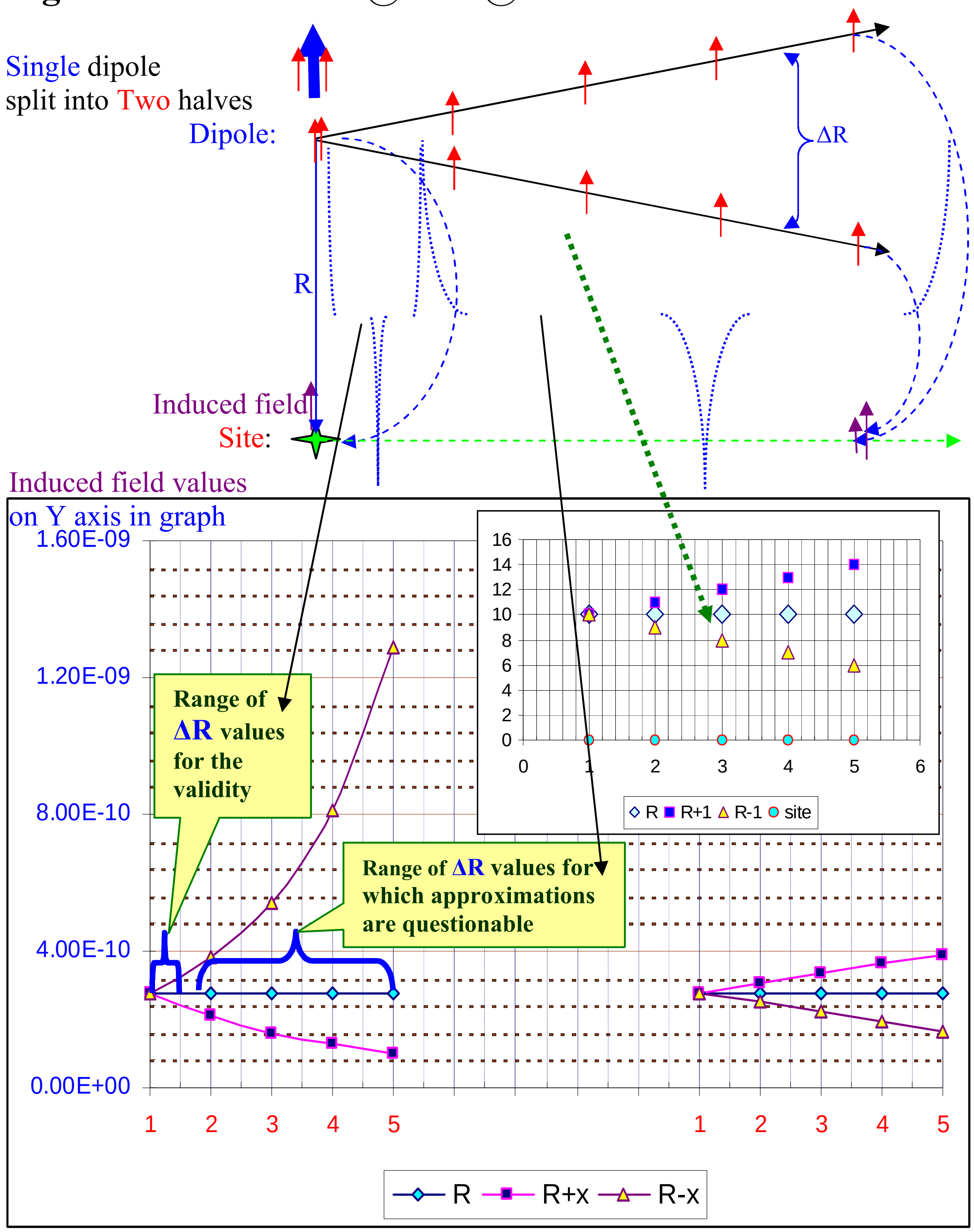
Isotropic Susceptibility Tensor

$$\tilde{\chi} = \begin{bmatrix} \chi & 0 & 0 \\ 0 & \chi & 0 \\ 0 & 0 & \chi \end{bmatrix} \qquad |\vec{R}| = r$$

$$\sigma_{zz} = \frac{\chi}{r^3} - \frac{3 \bullet r^2 \bullet \cos^2(\theta) \bullet \chi}{r^5}$$



For this equation, the variation of the contribution with distance for relative disposition of dipoles is graphically examined in the next Sheet.



The INSET in the graph above is schematically enlarged in the drawing above which indicates how the single dipole is split and placed to have the same average distance as the unsplit single dipole. Will the sum of contribution of the split halves be the same as the usplit single dipole? As seen in the left side of the graph, the contribution of the half placed below the average distance increases more rapidly with distance than the decrease of the contribution due to the half placed symmetrically above the average single dipole point. But even when two split halves are considered, the effective magnitude of the vectorially added halves is the same as the unsplit single dipole.

Materials given above in this SHEET should be added details to the considerations in SHEET-10 of the poster presented at the 6th NSC of the CRSI held in IIT/Kanpur during Feb. 2004: http://www.geocities.com/saravamudhan1944/crsi_6nsc_iitk.html

APPARENTLY CONFLICTING PRACTICES
An Observation

Thus the conclusion from the previous sheet should be that, when there is a magnetic moment which arises due to a circulation of electron charge cloud of finite size (not a point-charge) then the corresponding magnetic susceptibility would be attributed to be that of the entire extent (occupied region) of the charge cloud distribution. When dipole moment can be arising due to the presence of an external magnetic field, this cannot be a point-dipole. But the total magnitude of the dipole cannot be distributed uniformly over the region to further subdivide into smaller regions with proportionate dipole moment values to add up to the same total. This would not result in the same contribution to field distribution around as illustrated in the previous sheet. This is a severe constraint when the induced field distribution is considered relatively closer to the charge cloud and hence the criteria for the validity of point dipole approximation are in place to indicate the possible source and extent of of errors in estimates.

But when there are two **distinctly different** (*how can this distinction be attributed?*) charge cloud distributions it is a common practice to attribute two distinct dipole moments due to the charge clouds arising within the respective regions of the clouds. And, at an external point the induced fields from these two are estimated independently. *As per the arguments above, how is this situation different from placing two dipole moments split out from a single total dipole moment?* This is the criticality, for which a clarification is being presented in this contribution.

A RECONSIDERATION OF THE MATERIALS IN SHEET-0-7

The question of dividing a single dipole moment into smaller fragments and subsequent evaluation of the induced field contribution can be useful, if at a given distance from the original total dipole moment, the resulting induced field value is the same and does not result in ambiguities. The question of sub-dividing a dipole-fragment arises not because of the requirements of simplifying the equation used in the calculation methods. The purpose of such efforts to subdivide is to have better confidence in the calculated values and in any case the calculation method retains its simplicity to the same extent. The above means that the calculated induced field values must correspond to a physical entity which has validity, and should not be some easily calculated out number playing dubious role masking the reality from being transparent.

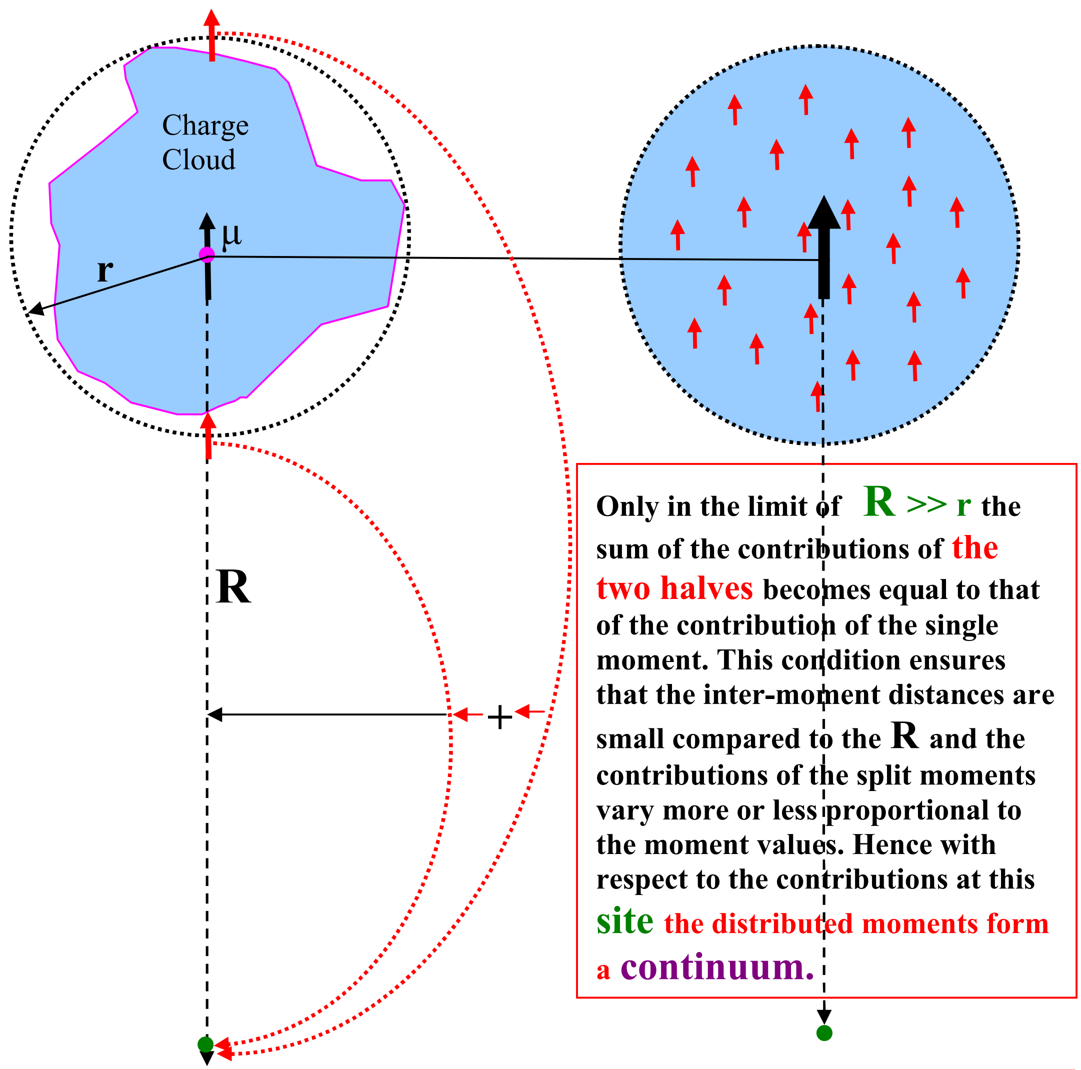
Obviously, when the subdivided elements are scattered closer to be confined within the region whose total size is significantly smaller than the distance to the site then the differences in the distances of various fragmented moments can all be negligibly small compared to the magnitude of the distance of the undivided total dipole moment. This is the condition, in other words, that the point dipole approximation should be valid.

Can there be criteria for the sub division which makes the point dipole approximations valid for the fragments better than retaining the dipole moment as the single total entity? Then this would result in a summed contribution for the total dipole moment within the validity critera of a point dipole. To look into the possibility of such criteria, the illustrations in the next sheet are in place.

As pointed out in Sheet_0_6 the induced filed contribution at a distance R from the dipole varies as $1/R^3$

Therefore the strength of the moment **μ** would be in the numerator, while the denominator would have the factor $\mathbf{R}^3$

The charge cloud which gives rise to this dipole moment is confined to a region which can be included completely within a sphere of minimum radius ‘r’, then the pictorially this situation can be envisaged as follows.



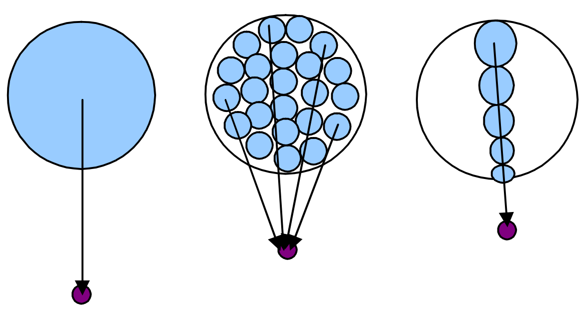
This is the detailed perspective of the contents on sheet_0_3 and sheet_0_7 and also explains why for demagnetization factors considering **discrete** distribution of magnetic moments would not be possible. That would be a question of calculating contributions from points within the cloud-region at a point within the same region. The type of condition as above cannot be realized.

INNOVATIVE solution?

How to circumvent the constraints which were enumerated in the previous illustrations?
This question can be reformulated as below:

> When there is a Charge cloud in a region of radius **r** and with an assigned total susceptibility χ, then how can the induced field contributions can be calculated at much closer (**smaller R values**) distances to this charge cloud by considering a discrete set of moments totaling to the single undivided moment?

In order that the point-dipole approximation be valid for the divided moments, the total charge cloud region must be considered as being divided into close-packed smaller cloud regions. Then, the conventional trial would be the simple division into equal parts. Then the 'r' values concerned become significantly smaller but the distance R can also be made correspondingly smaller while considering contribution from individual divided elements. As R becomes smaller and the site closer to the total region, the R becomes relatively smaller compared to the radius r_t for the total region. Hence the total contribution would not be the same as what it would be for the single undivided moment placed at the centre of the region. More over the entire charge cloud region must be closely packed with the divided element to take proper account of the material and the volume it occupies. There can be simpler way to go about close filling and summing the contribution if the divided fragments are allowed to vary in size depending on their distance from the site.



As the site gets closer and closer, the divided element at the near edge of the region also can be made smaller and smaller for the point dipole approximation to be valid and let this size increase within the totality of the region.

In fact, if the point dipole approximation is made valid to a better extent than with a single undivided element, the resulting sum of the contribution would not be the same as the value calculated for the undivided moment. If the pint dipole approximation did not break down in this process then the resulting summed value must be closer to the true contribution of the charge cloud at that closer distance. By applying this criterion to the induced field within the specimen itself, the demagnetization factors would result and there are well tabulated standard values for this physical quantity and which can be used for standardizing this procedure.

Such were the considerations which have been documented in the following websites:

1. http://saravamudhan.tripod.com/
2. http://nehuacin.tripod.com
3. http://www.geocities.com/saravamudhan1944/crsi_6nsc_iitk.html
4. http://www.geocities.com/inboxnehu_sa/crsi_nsc8_iitb.html

The case of single crystals presents the converse also to be true.

The single crystal specimen consists of only discretely placed molecules with each molecule having well defined positional coordinates. When the molecular dimension becomes smaller with respect to the distance of point where its induced field contribution is calculated, and further the intermolecular distances are also small, then the molecular susceptibilities can be combined (opposite of the dividing process mentioned earlier/ the possible continuum) into a larger entity. This would reduce the number of summation to be made and hence reduce the calculation time. This would make such a difference that what was an impossible number of elementary summation to be calculated, would become a matter of pocket calculation. The HR PMR in single crystalline solid state is the case of where the induced fields from the discrete region, the continuum are all relevant as much as the induced fields due to electron charge cloud circulation within the individual molecule. This relevance had been highlighted in the contribution at the NSC8, IIT/Bombay as documented in the webpage no:4 listed above.

Also find relevant materials in the content of:
http://nehuacin.tripod.com/pre_euromar_compilation/id5.html

More specific to this theme of "continuum and discreteness" find a slide show (CMDays2006) uploaded in the webpage
http://nehuacin.tripod.com/id1.html at the link for MRSFall2006